Another Bayesian Analysis of the Thermal Challenge Problem

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In this talk we describe the types of problems we work with at Los Alamos National Laboratory and how we see these problems fitting into the framework described in the tasking document for this workshop. We briefly describe tools and methods we have developed that utilize experimental data and detailed physics simulations for uncertainty quantification. Finally, we apply these tools to the thermal challenge problem. This statistical framework used here is based on the approach of Kennedy and O'Hagan (2001), but has been extended to deal with functional output of the simulation model.

LA-UR-06-3657

Thermal Validation Challenge Problem: GPM solution

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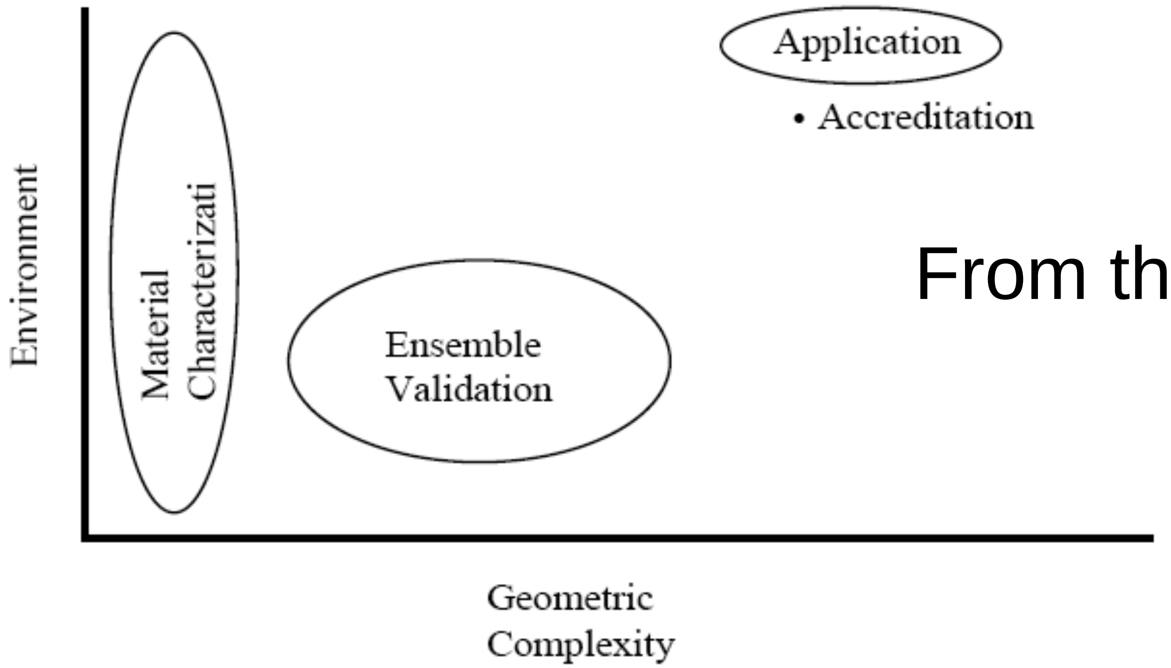
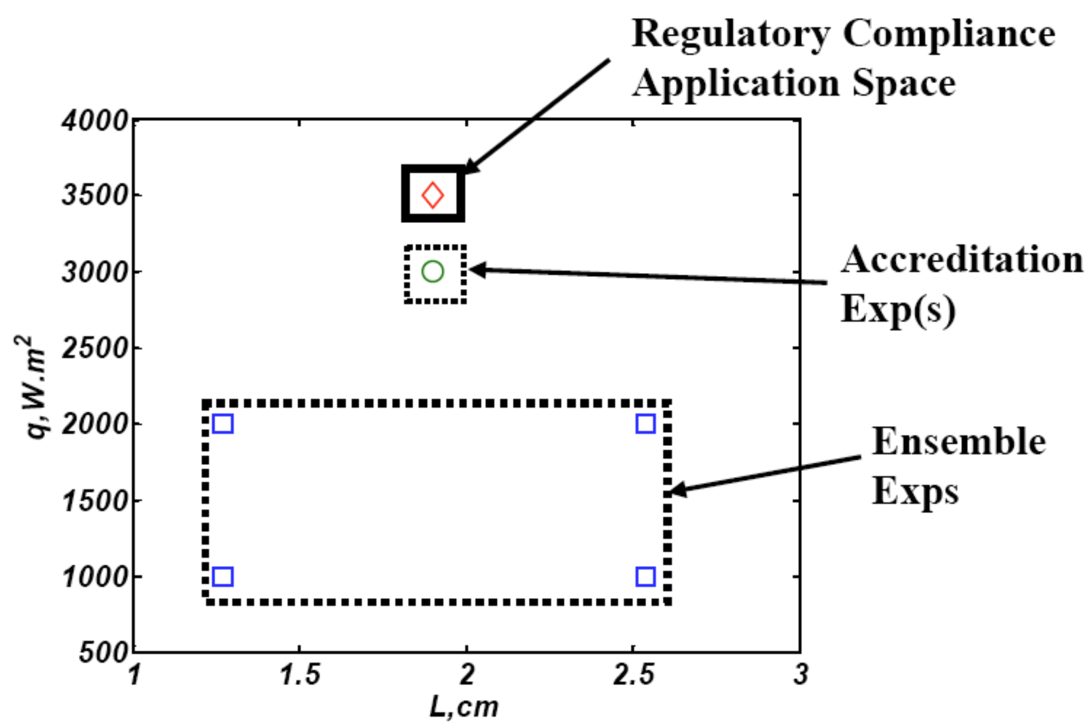
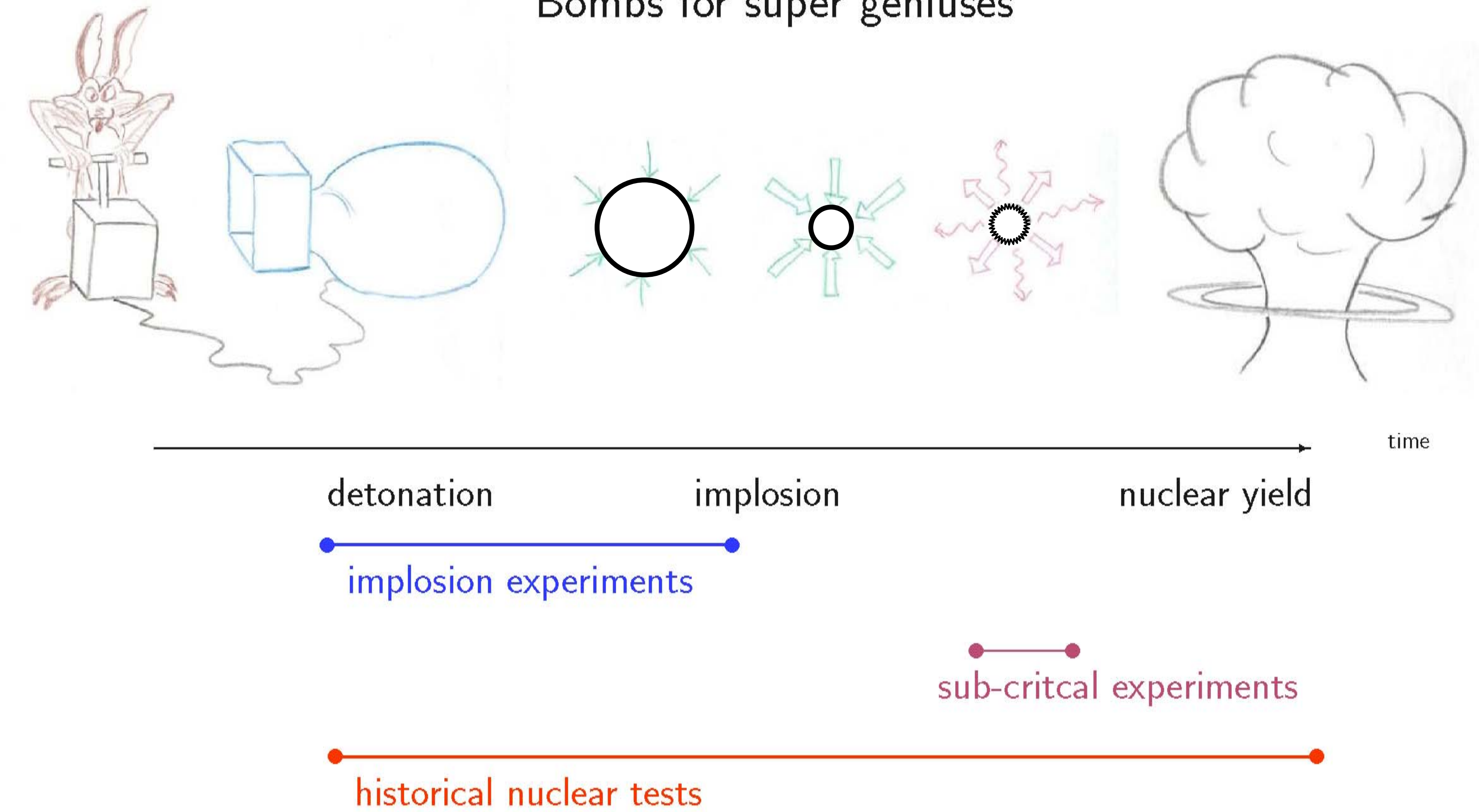
From the tasking document





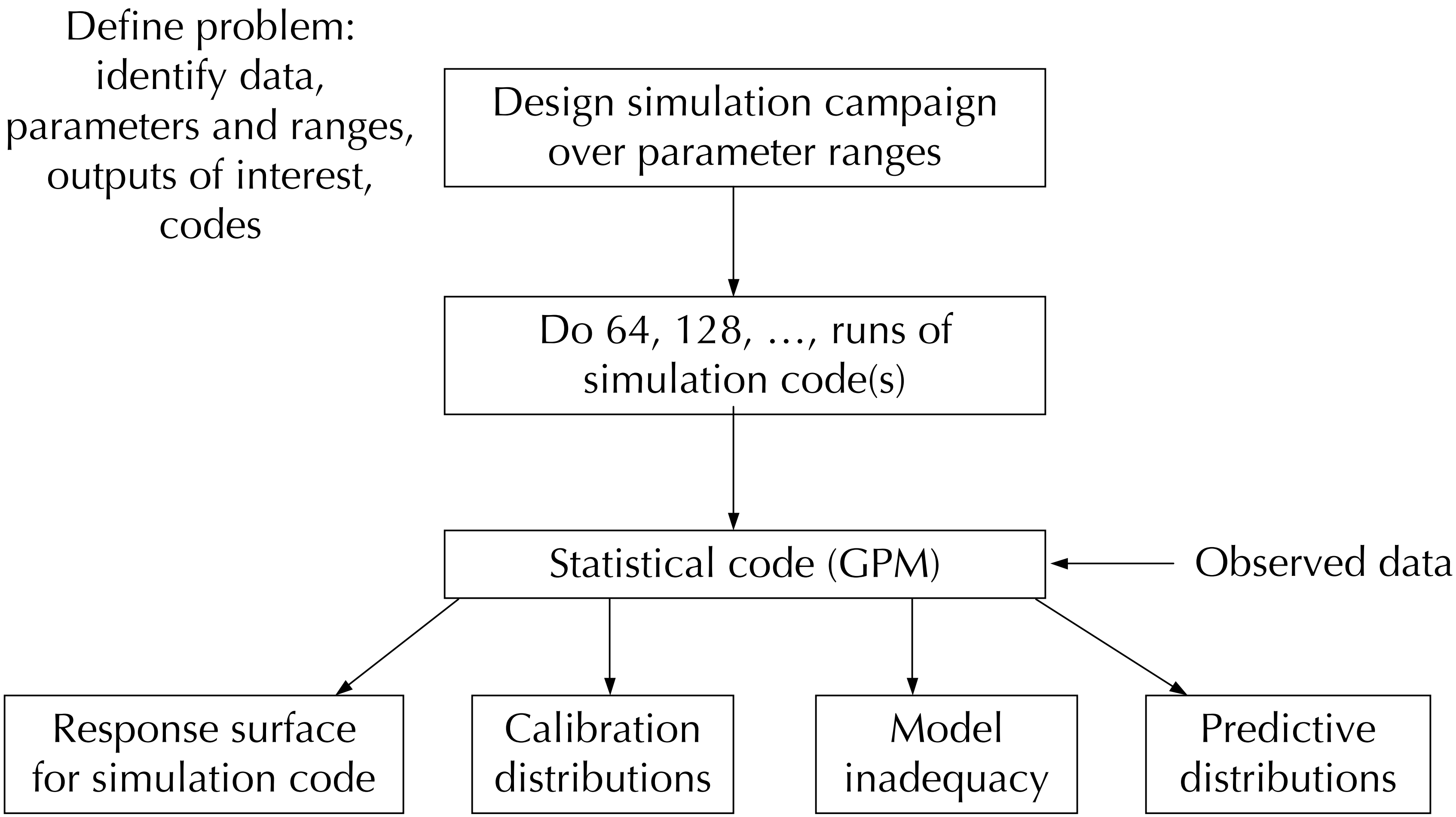
Certification Issues at LANL

Bombs for super geniuses

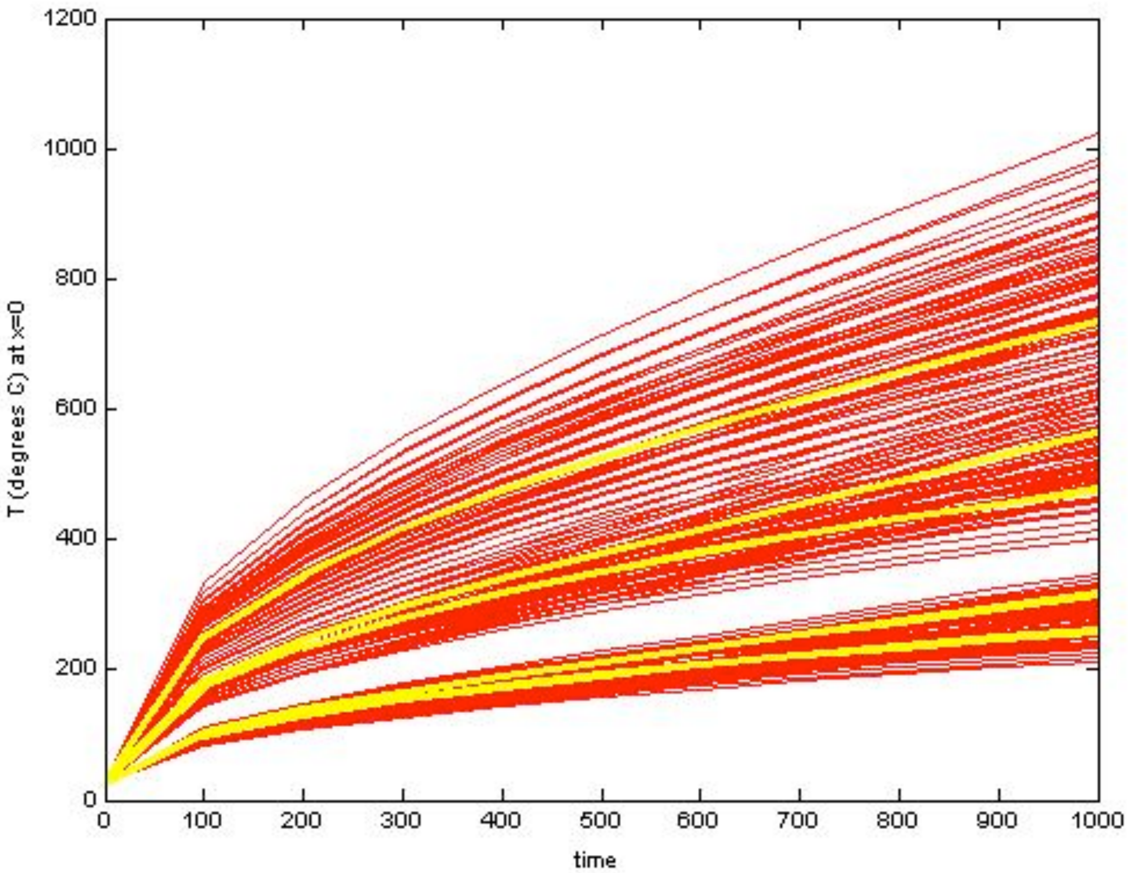


off-line experiments
materials, equations of state (EOS), high explosive (HE)

Our analyses use statistical methods to combine different simulation codes and observational data



Uncalibrated sims and calibration data

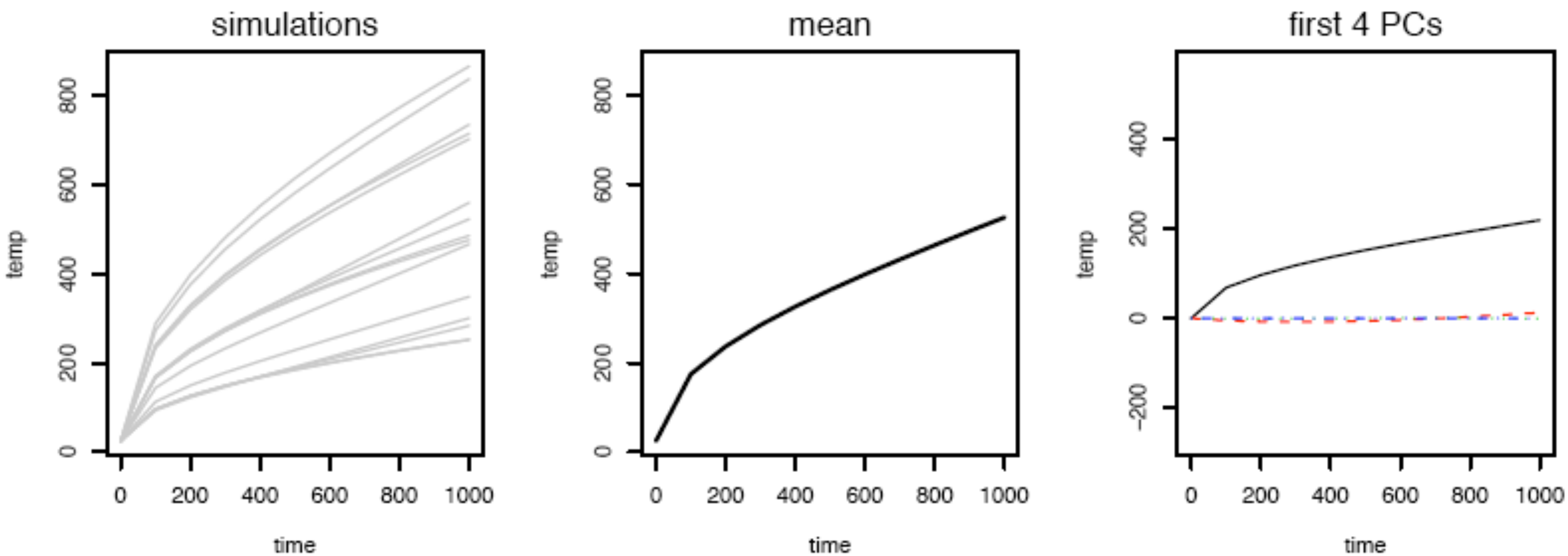


36 x 6 simulations

A single experiment for each configuration (1-5).

Basis representation of simulated profiles

The temperature profiles resulting from the 216 simulations are used to construct a mean-adjusted principal component representation.



Temperature profiles are represented as a function of the 4-d input parameters (x,θ) and PC basis functions $\phi_j(t)$:

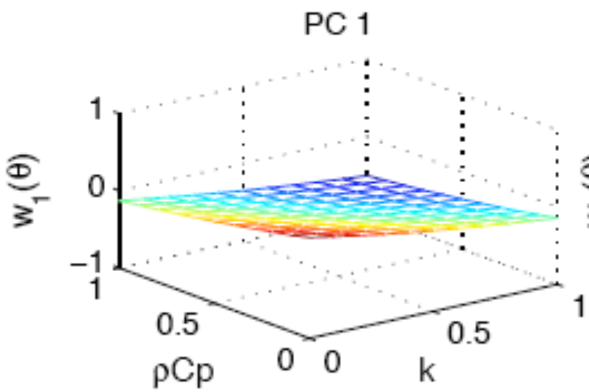
$$\widehat{\eta}(x,\theta;k) = \sum_{j=1}^{p_\eta} w_j(x,\theta)\phi_j(t)$$

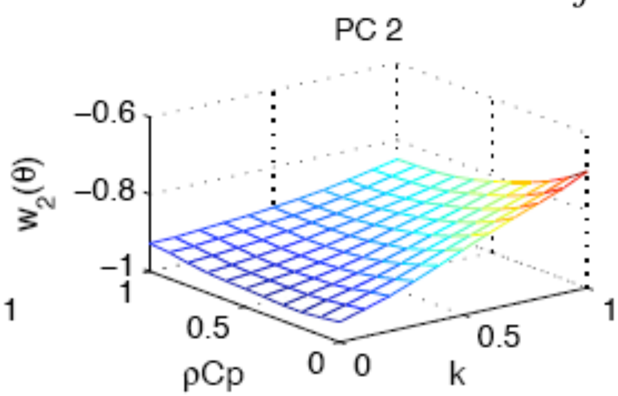
Gaussian process model to *emulate* simulation output

Gaussian process (GP) models are used to estimate the weights $w_j(\theta)$ at untried settings

$$\widehat{\eta}(x,\theta;k) = \sum_{j=1}^{p_\eta} w_j(x,\theta)\phi_j(t)$$

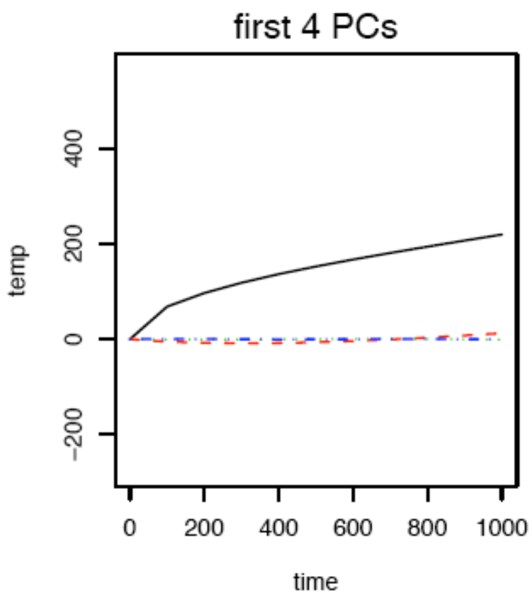
GP models $w_j(x,\theta)$



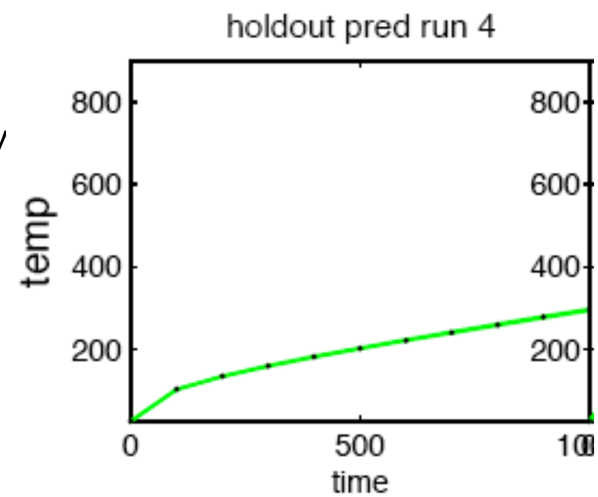


x set to Config 4

Bases $\phi_j(x,\theta)$

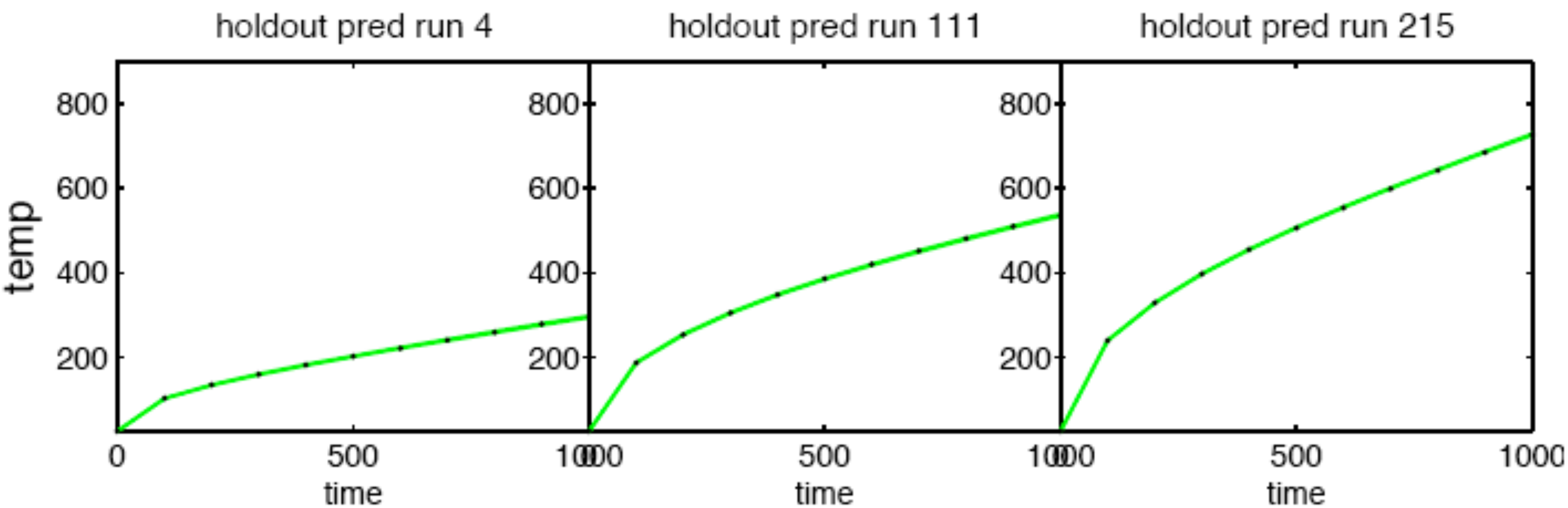


Prediction at new

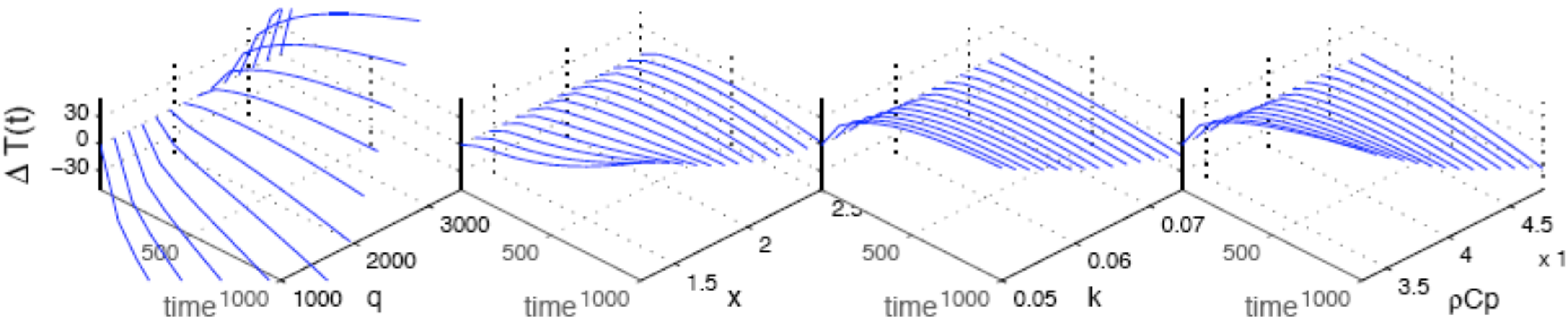


Checking the emulator

Errors ~ 0-3^{o}C



Simulator emulation and sensitivity



Changes in the emulator prediction as each parameter is varied while holding the others at their midpoint.

Note: k and ρCp have a similar effect on Temperature

Model of the data

$$y(t) = \eta(x, \theta; t) + \delta(x; t) + \epsilon_{rep}(t)$$

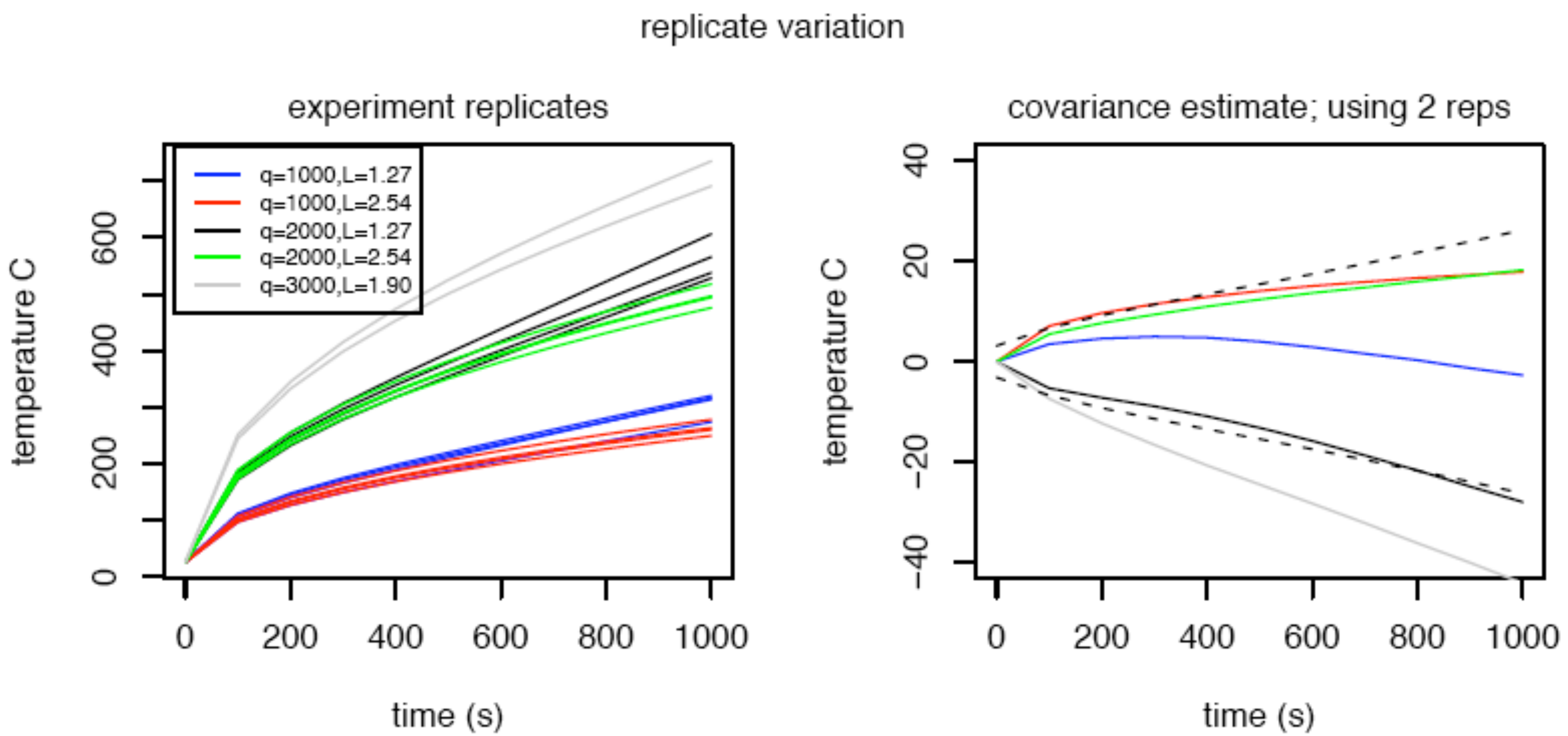
Posterior density:

$$\pi(\delta(\cdot; t), \eta(\cdot, \cdot; t), \theta, \xi | y) \propto L(y | \delta(\cdot; t), \eta(\cdot, \cdot, t), \theta, \Sigma_\epsilon)$$
$$\times \pi(\delta(\cdot; t) | \xi) \times \pi(\eta(\cdot, \cdot; t) | \xi) \times \pi(\theta) \times \pi(\xi)$$

Σ_e is known, ξ controls statistical parameters governing $\eta(\cdot, \cdot; t)$, $\delta(\cdot; t)$, and Σ_e.

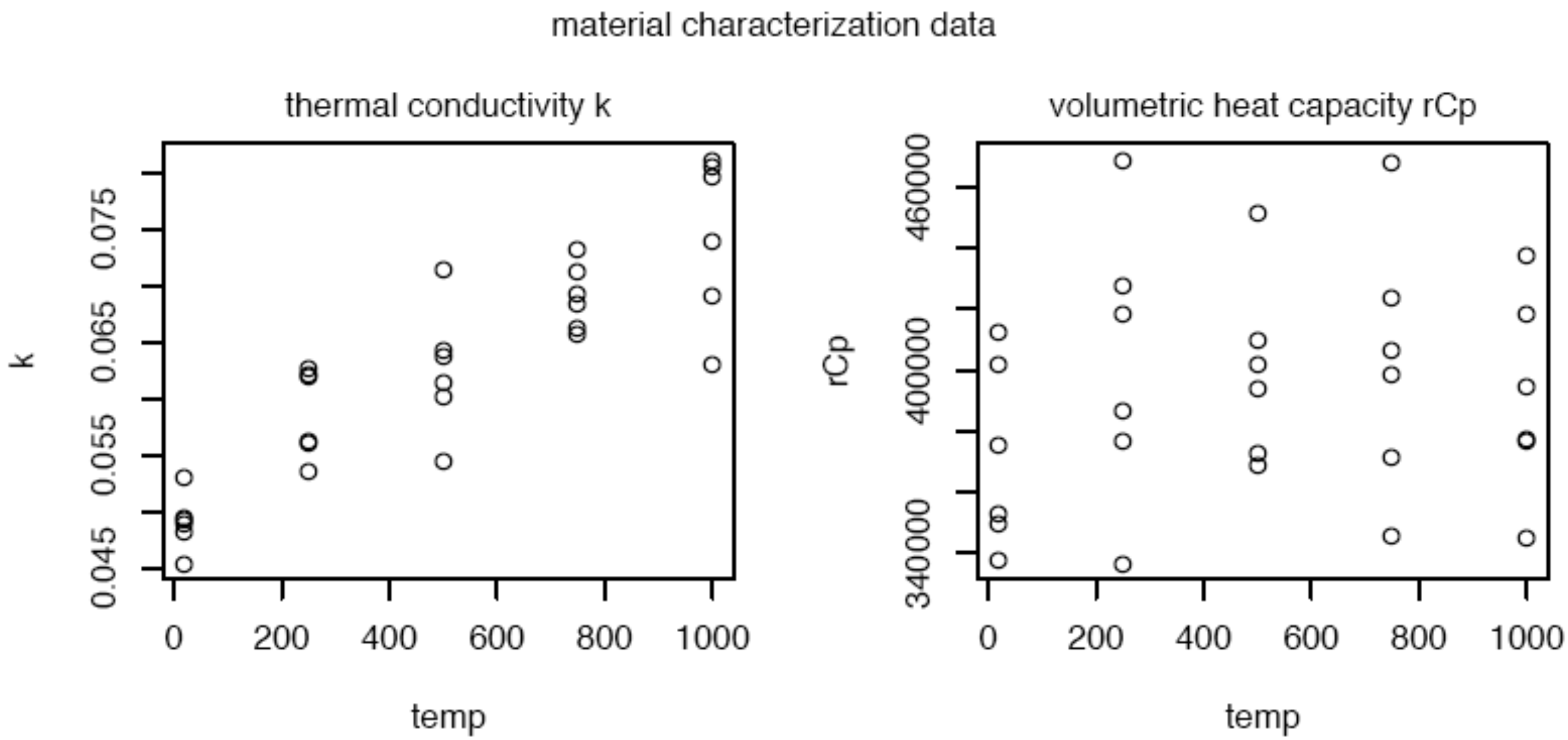
Posterior for distributions/integrals computed via MCMC

Modeling replicate variation



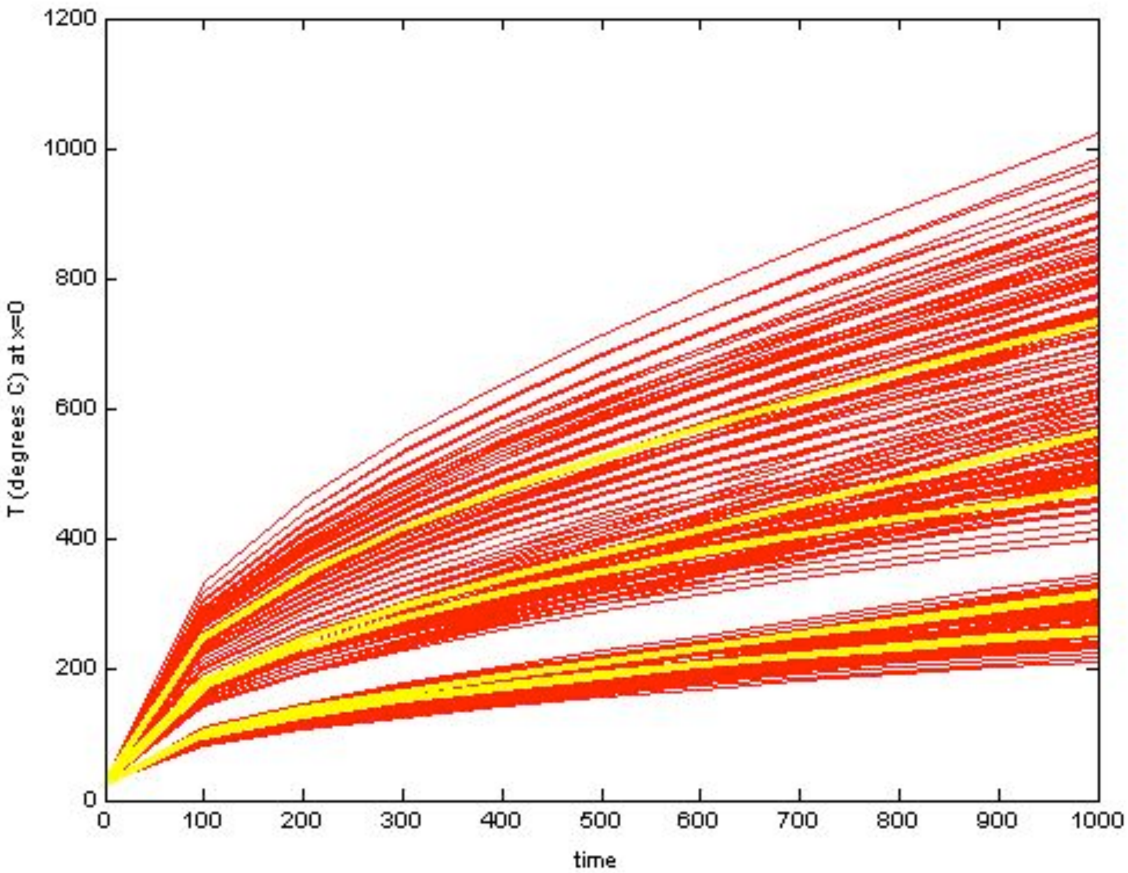
Correlated model for Σ_e

Use of material characterization data



Gives initial range for calibration

Using 1 experiment from 4 configurations

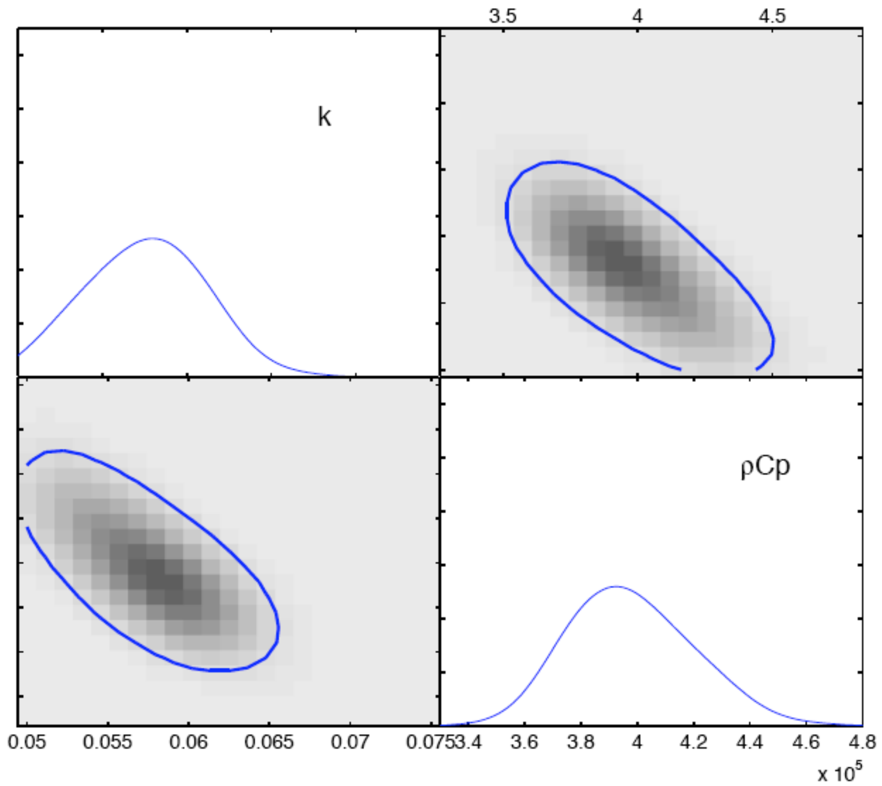


Similar to many LANL applications

Can assess our prediction for the Accreditation experiment

Gives an idea of whether we can trust extrapolations

1st analysis: using only a single expt from the 4 configurations



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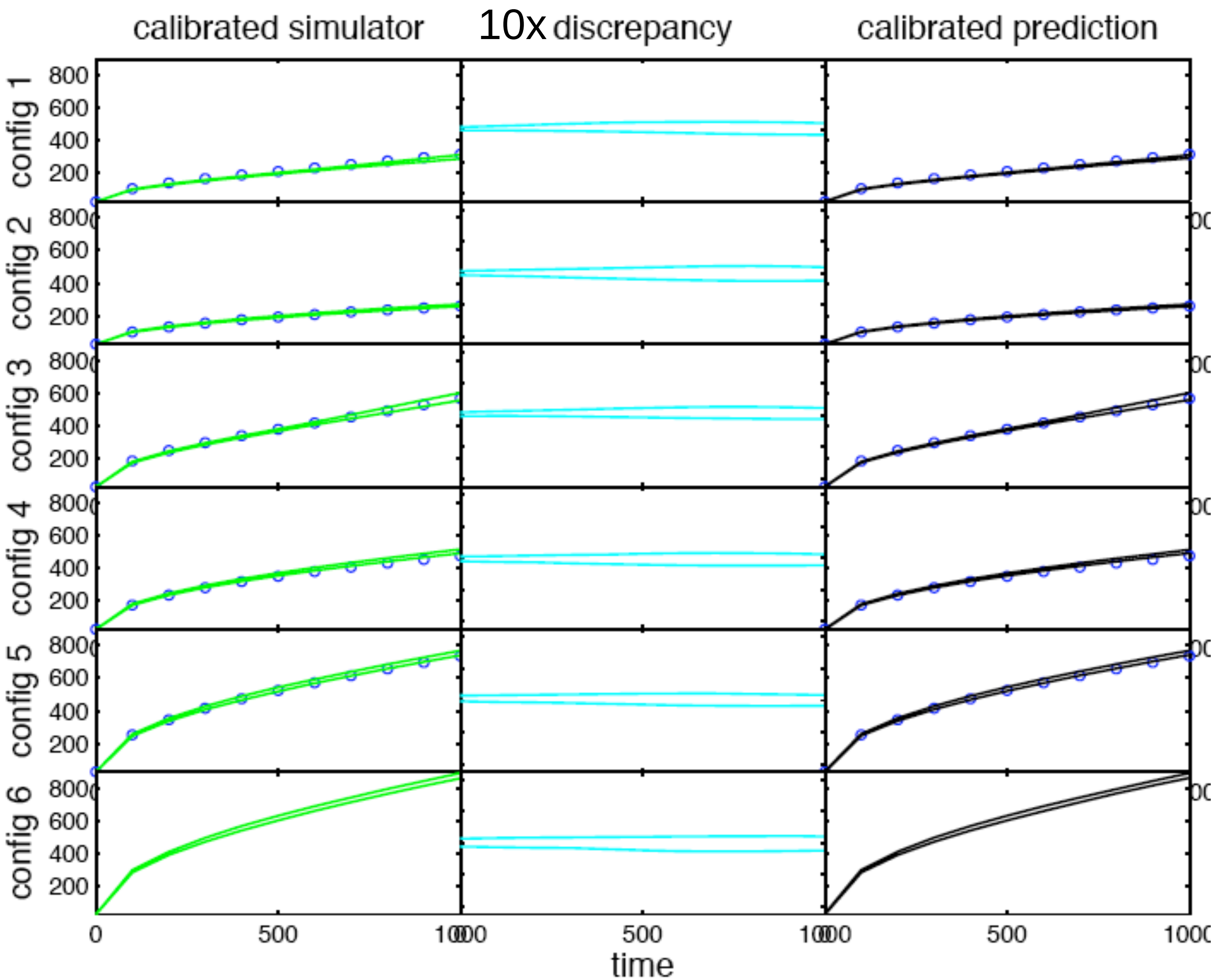

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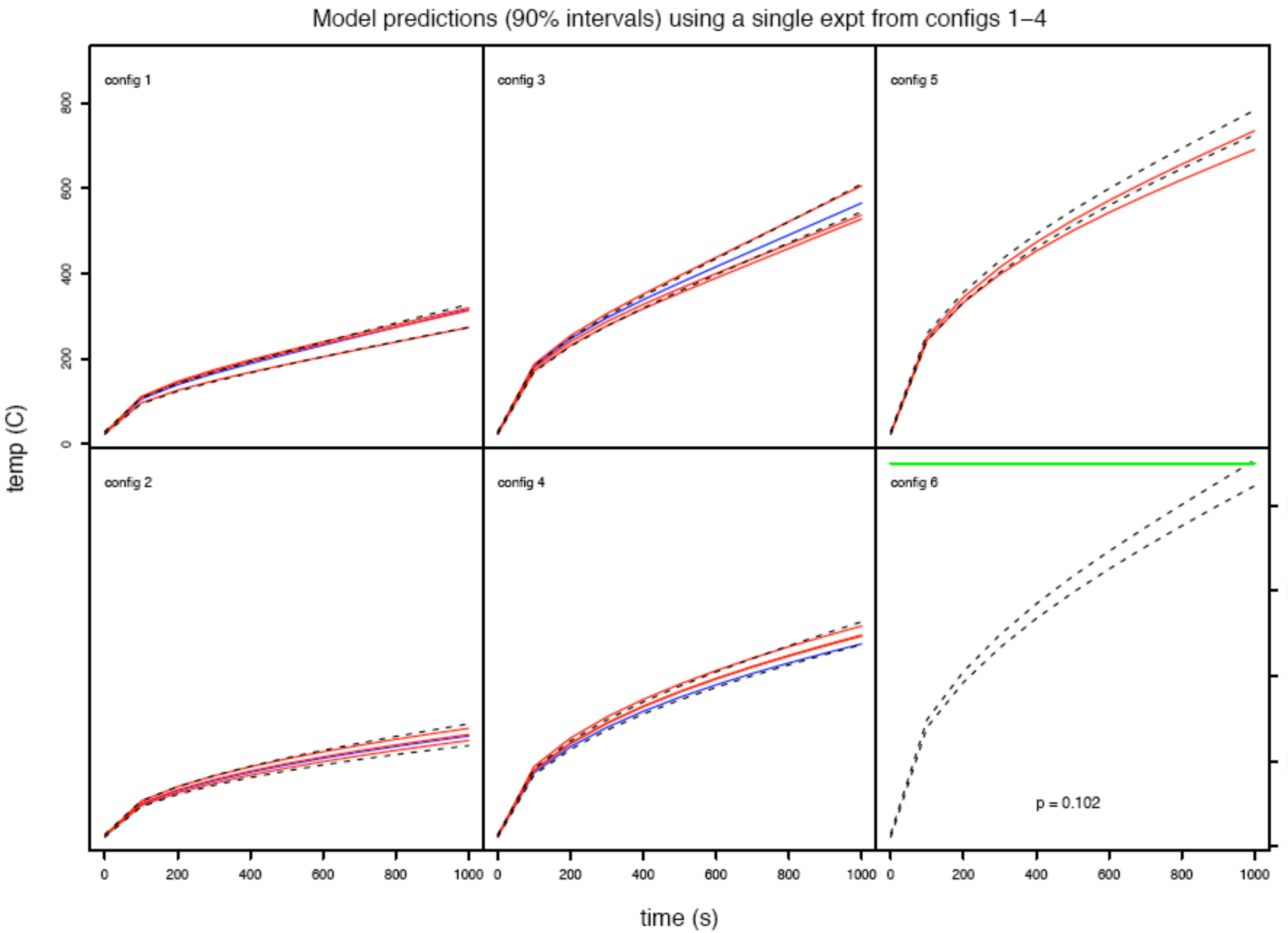
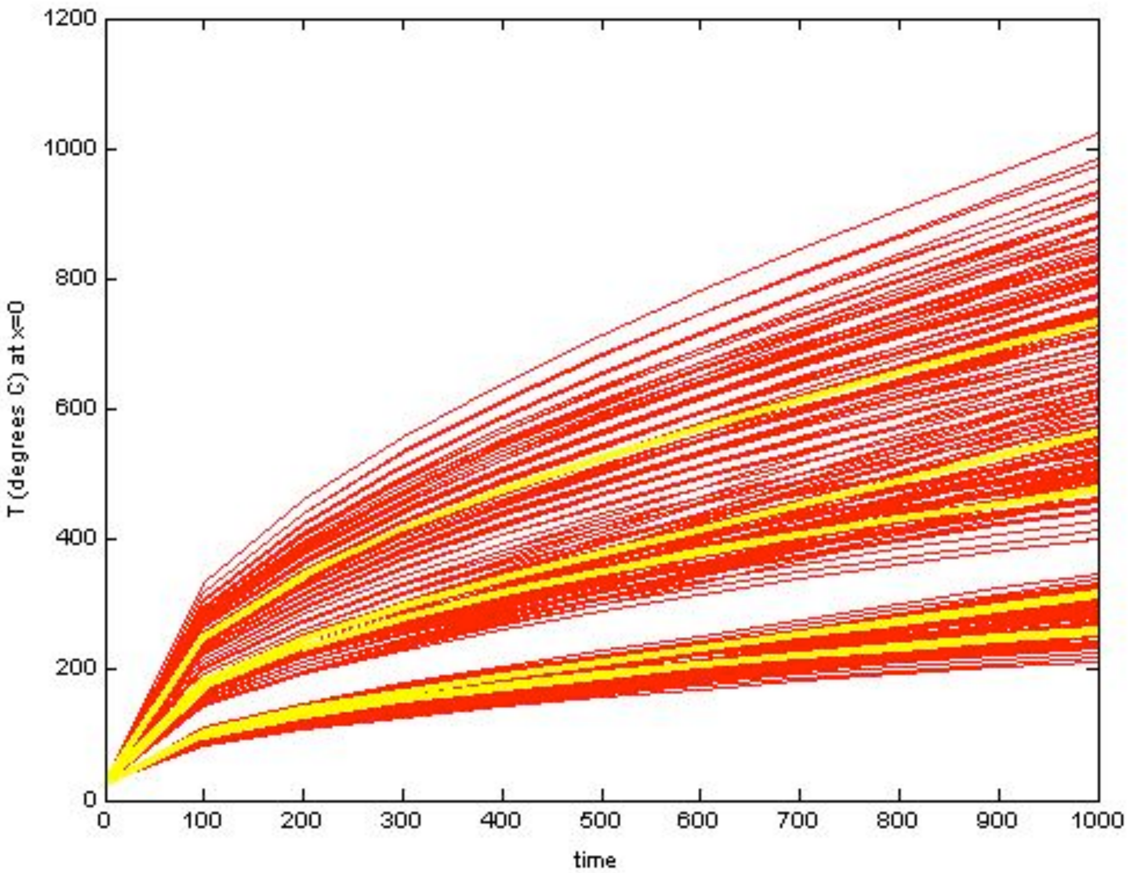


Using 1 experiment from 4 configurations + 1 accreditation expt



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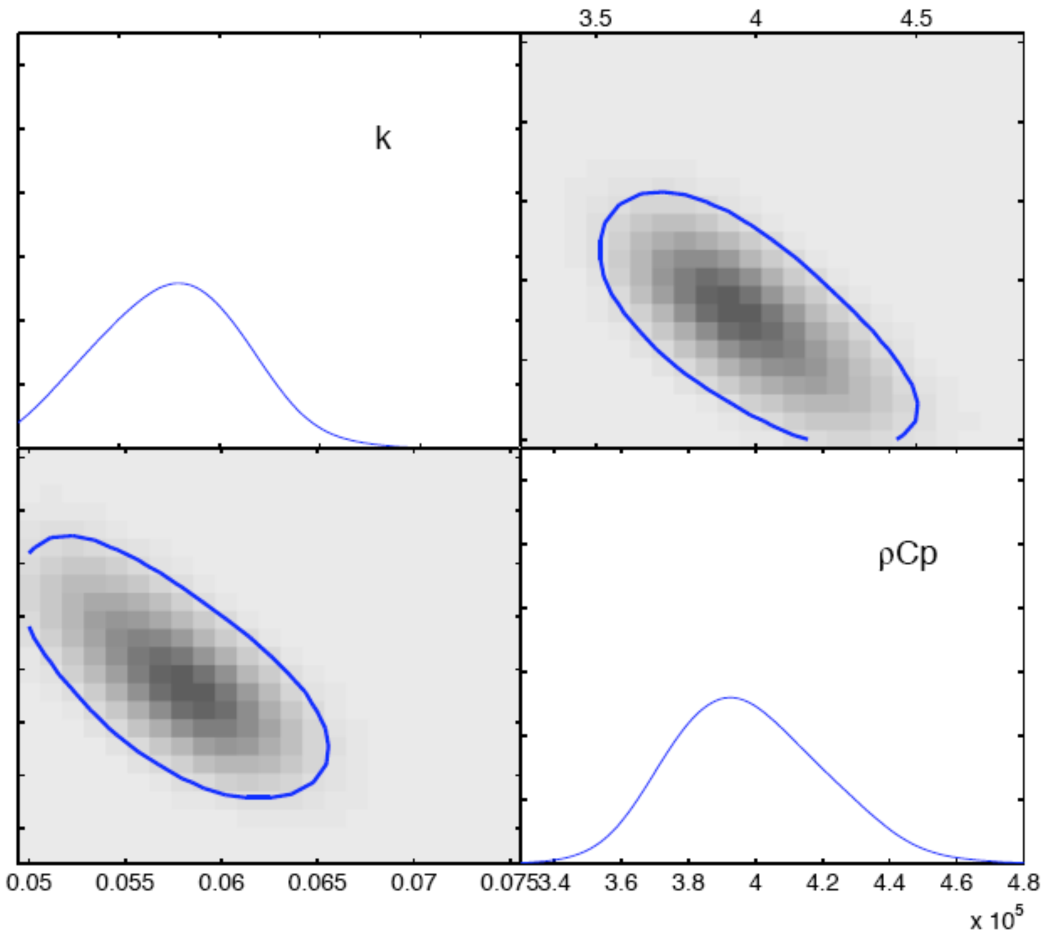
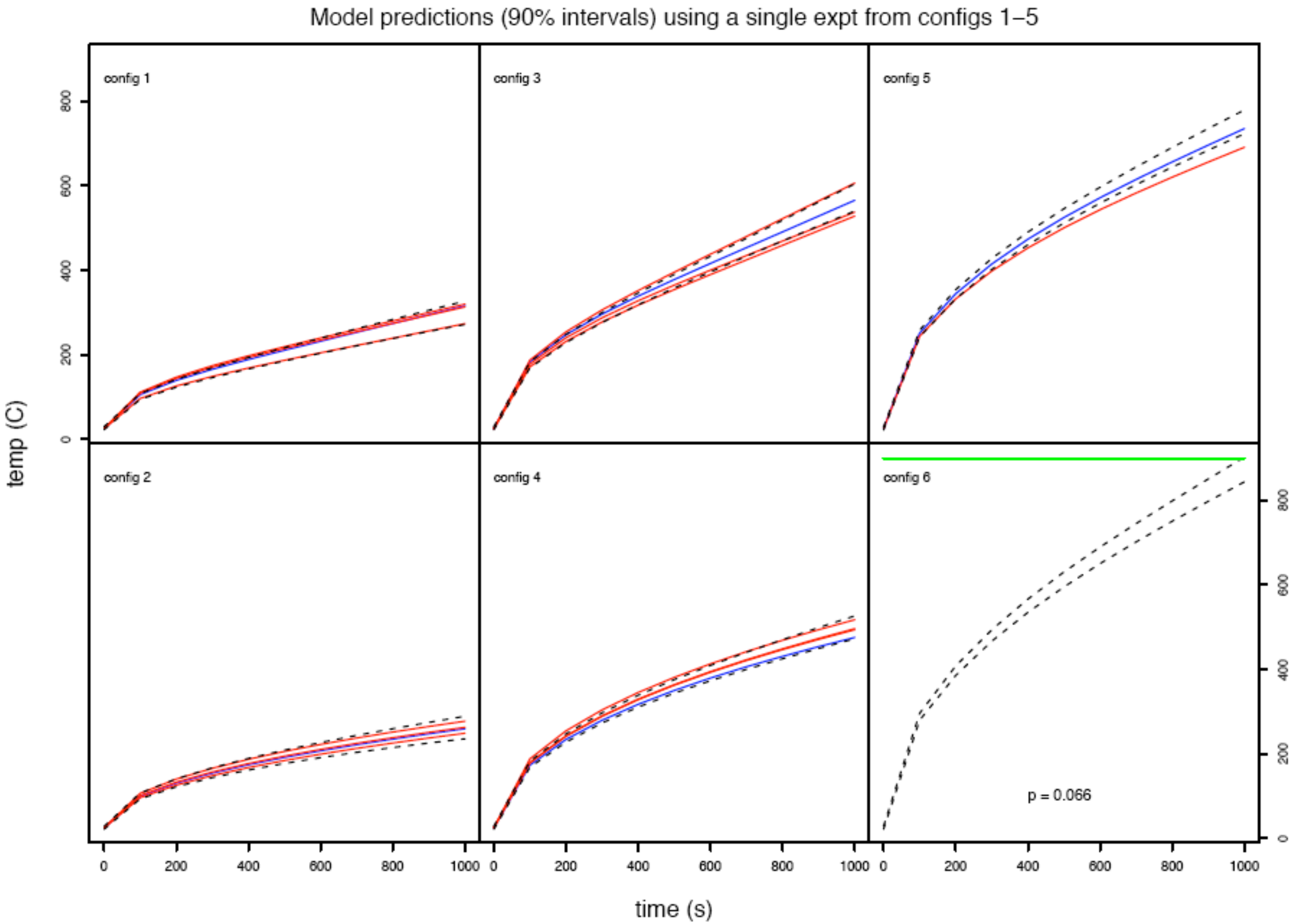
2nd analysis: 4+1 expts



2nd analysis: 4 + 1 expts



Discussion

- here, tail behavior of replicates important
- "reach" of constituent models in simulation models crucial for extrapolation
- Assessing trust in answers: experts, subject matter, holdout predictions, test statistics(?)
- Discrepancy model building with experts
- Metrics and discrepancy
- Focus on major sources of uncertainty and heartburn
- Philosophy: use all info at hand.
- Coupling multiple types of experiments